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AN EFFICIENT WEAK LINE SEARCH WITH GUARANTEED TERMINATION.(U)

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M. R. Osborne

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Mathematics Research Center
University of Wisconsin—Madison
610 Walnut Street
Madison, Wisconsin 53706

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AN EFFICIENT WEAK LINE SEARCH WITH GUARANTEED TERMINATION

M. R. Osborne

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ABSTRACT

A method based on repeated quadratic interpolation is proposed for satisfying a weak line search criterion given by A. A. Goldstein and it is shown to be efficient and to have guaranteed termination. An extension of the line search criterion appropriate to minimum norm problems is sketched.

AMS (MOS) Subject Classifications: 65D05, 65H10, 65K05

Key Words: Unconstrained minimization, Nonlinear equations, Descent algorithms, Line search, Interpolation.

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SIGNIFICANCE AND EXPLANATION

Many algorithms for the minimization of functions use iterative procedures that first choose a search direction, and then decide how far to proceed along the search direction. These methods rely heavily on the availability of a standard procedure to control the length of step taken at each iteration. This report describes one possible such procedure which is both efficient and has guaranteed termination. It also has the advantage that it requires only function values to carry out the line search, although it applies in general only to methods which compute derivatives in estimating the search direction.

Computational experience has been very satisfactory over a number of years, and on average little more than one function value needs to be computed at each step. Also the basic ideas of the line search test have been adapted to minimum norm problems of which one important particular case is Newton's method. Here, provided the search directions are bounded and the singularities of the Jacobian isolated, then limit points of the iteration are solutions to the nonlinear system. The boundedness condition on the search direction can not be relaxed.

The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the author of this report.

AN EFFICIENT WEAK LINE SEARCH WITH GUARANTEED TERMINATION

M. R. Osborne

1. Introduction.

In descent methods for minimization and in the use of descent steps to stabilize methods for the solution of nonlinear equations the computation characteristically falls into two parts: the determination of a direction of descent, and then a line search to estimate the length of step in this direction. This paper is addressed to the second question.

Methods for determining the length of step are of two main types: those which compute the step as an estimate of the distance to the minimum in the descent direction, and those which are satisfied if the step achieves a significant reduction in the function value. The first kind of line search fitted well with the development of conjugate direction algorithms where conceptually important theoretical information is available when the exact minimum is computed. In general the approach used in these methods is to fit an interpolating function (typically a quadratic or cubic polynomial) to the most recent information, compute the minimum of this interpolant, and use this as a new estimate of the minimum. Methods of this kind are discussed in [1], and recently Robinson [7] has pointed out problems with repeated quadratic interpolation. However, these methods are usually significantly less efficient in the sense that they force more function values over all than methods of the second type (the weak line search methods). Our purpose here is to give an efficient implementation with guaranteed termination for satisfying a weak line search criterion due to Goldstein [3].

To specify this criterion let $F: R_n \to R_1$ be the function to be minimized. At the current point $\underset{\sim}{x}$ the descent algorithm generates the vector $\underset{\sim}{h}$ determining the descent step. It is assumed that $\underset{\sim}{h}$ is downhill which means that $\exists \delta > 0$ such that

$$\nabla F(\underset{\sim}{x})\underset{\sim}{h} \leq -\delta \|\nabla F(\underset{\sim}{x})\| \, \|\underset{\sim}{h}\| \tag{1.1}$$

$\forall \underset{\sim}{x} \in R$ where R is a region containing the successive iterates, also that F is bounded below on R, and that $F \in C^2(R)$. The exact specification of the norm in (1.1) is not important. Let

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$$\psi(\underset{\sim}{x}, \underset{\sim}{h}, \lambda) = -\frac{F(\underset{\sim}{x}) - F(\underset{\sim}{x} + \lambda\underset{\sim}{h})}{\lambda \nabla F(\underset{\sim}{x})\underset{\sim}{h}} \quad . \tag{1.2}$$

Initially we try a preset value λ_0 (although there would likely also be a test on $\|\underset{\sim}{h}\|$ to ensure that $\lambda_0 \underset{\sim}{h}$ is not too large), and accept this if

$$0 < \sigma \leq \psi(\underset{\sim}{x}, \underset{\sim}{h}, \lambda) \tag{1.3}$$

with $\lambda = \lambda_0$. If this test fails we seek a λ satisfying both (1.3) and

$$\psi(\underset{\sim}{x}, \underset{\sim}{h}, \lambda) \leq 1 - \sigma \quad . \tag{1.4}$$

Clearly we must choose $\sigma < 1/2$ and usually it is taken small (say 10^{-4}).

Remark (i). It is important to note that the Goldstein procedure is not usually appropriate if derivatives of F are not available unless an alternative to a difference calculation is available to compute $\nabla F(\underset{\sim}{x})\underset{\sim}{h}$ (an example is indicated in section 4.).

(ii) The significance of ψ can be seen by noting that it relates the decrease in F in the step λ to the decrease that would be observed if F were linear. The Goldstein test imposes a sense in which these two quantities are comparable. For this reason it is not surprising that it has proved very useful both in the analysis and implementation of algorithms using function and first derivative information.

2. Properties of the Goldstein test.

The basic assumption made on F is that it can be expanded in the form

$$F(\underset{\sim}{x} + \lambda\underset{\sim}{h}) = F(\underset{\sim}{x}) + \lambda \nabla F(\underset{\sim}{x})\underset{\sim}{h} + \lambda^2 \|\underset{\sim}{h}\|^2 \int_0^1 (1-s)F''(\underset{\sim}{x} + (\lambda\underset{\sim}{h})s)\,ds \tag{2.1}$$

where the ' indicates differentiation in the direction defined by $\underset{\sim}{h}$ which is assumed bounded. We now give two key properties which follow from the form of the test and which are basic to its usefulness.

(i) For each $\underset{\sim}{x}$, and for $\underset{\sim}{h}$ satisfying (1.1), then either $\nabla F(\underset{\sim}{x})\underset{\sim}{h} = 0$ or $\exists\, \lambda$ such that either $\lambda = \lambda_0$ satisfies (1.3) or $\exists \lambda$ satisfies (1.3) and (1.4).

(ii) For any algorithm producing directions satisfying (1.1) applied to F where F has bounded second derivatives in R then limit points of the sequence of iterates $\{\underset{\sim}{x}_i\}$ are points at which $\nabla F(\underset{\sim}{x})\underset{\sim}{h} = 0$.

To show (i) we have

$$\psi(\underset{\sim}{x}, \underset{\sim}{h}, \lambda) = 1 - \frac{\lambda\|\underset{\sim}{h}\|}{|F'(\underset{\sim}{x})|}\int_0^1 (1-s)F''(\underset{\sim}{x} + (\lambda\underset{\sim}{h})s)ds \tag{2.2}$$

$$\to 1, \ \lambda \to 0 \quad \text{for fixed} \quad \underset{\sim}{x}, \underset{\sim}{h} \ .$$

To show (ii) note that if the sequence of step lengths $\{\lambda_i\}$ satisfies $\{\lambda_i\} \geq \bar{\lambda} > 0$ then (1.3) implies that

$$-\nabla F(\underset{\sim}{x}_i)\underset{\sim}{h}_i \leq \frac{1}{\bar{\lambda}\sigma}\{F(\underset{\sim}{x}_i) - F(\underset{\sim}{x}_{i+1})\} \tag{2.3}$$

and the result follows from this as the sequence $\{F(\underset{\sim}{x}_i) - F(\underset{\sim}{x}_{i+1})\}$ is decreasing and bounded below. It follows from (2.2) that $\lambda_i > 0$ for any particular $\underset{\sim}{x}_i$, $\underset{\sim}{h}_i$. Thus $\bar{\lambda} = 0$ if and only if $\exists$ subsequence $\{\lambda_{\nu_i}\} \to 0$. It is the second test (1.4) which ensures that λ does not get too small in the set of allowable values for each $\underset{\sim}{x}$, $\underset{\sim}{h}$. Here it gives (using (2.2))

$$1 - \frac{\lambda_{\nu_i}\|\underset{\sim}{h}_{\nu_i}\|}{|F'(\underset{\sim}{x}_{\nu_i})|}\int_0^1 (1-s)F''(\underset{\sim}{x}_{\nu_i} + (\lambda_{\nu_i}\underset{\sim}{h}_{\nu_i})s)ds \leq 1 - \sigma$$

which implies that

$$|F'(\underset{\sim}{x}_{\nu_i})| \leq \frac{\lambda_{\nu_i}\|\underset{\sim}{h}_{\nu_i}\|}{\sigma}\int_0^1 (1-s)F''(\underset{\sim}{x}_{\nu_i} + (\lambda_{\nu_i}\underset{\sim}{h}_{\nu_i})s)ds \tag{2.4}$$

and the result follows from this and the assumed boundedness of $\|\underset{\sim}{h}\|$.

The conditions under which $\nabla F(\underset{\sim}{x})\underset{\sim}{h} = 0 \Rightarrow \underset{\sim}{x}$ is a stationary point of F require a deeper study of the particular descent algorithm. However, if the downhill condition holds then this implies either $\|\nabla F(\underset{\sim}{x})\| = 0$ or $\|\underset{\sim}{h}\| = 0$, and the problem is reduced to ruling out cases in which the second condition holds and $\|\nabla F(\underset{\sim}{x})\| \neq 0$. One class of methods for which this can be done simply is the class related to steepest descent in the sense that the downhill condition can be stated in the form

$$\nabla F(\underset{\sim}{x})\underset{\sim}{h} \leq -\frac{1}{\delta}\|\nabla F(\underset{\sim}{x})\|^2 \ . \tag{2.5}$$

Clearly limit points are points at which $\|\nabla F(\underset{\sim}{x})\| = 0$ in this case.

3. A line search strategy.

In this section a procedure for satisfying (1.3) and (1.4) is given which is both efficient and has guaranteed termination. The procedure is as follows. If at the current stage of testing λ_k fails either (1.3) or (1.4) with $k > 0$ then:

(i) If λ_k fails (1.3) so that

$$F(\underset{\sim}{x} + \lambda_k \underset{\sim}{h}) > F(\underset{\sim}{x}) - \sigma\lambda_k \|\underset{\sim}{h}\| F'(\underset{\sim}{x}) > F(\underset{\sim}{x}) \tag{3.1}$$

then form the quadratic interpolation polynomial

$$\phi_k(\lambda) = F(\underset{\sim}{x}) + \lambda\|\underset{\sim}{h}\|F'(\underset{\sim}{x}) + \lambda^2\|\underset{\sim}{h}\|^2 C_k \tag{3.2}$$

where C_k is determined by

$$\phi_k(\lambda_k) = F(\underset{\sim}{x} + \lambda_k \underset{\sim}{h})$$

giving

$$C_k = (F(\underset{\sim}{x} + \lambda_k \underset{\sim}{h}) - F(\underset{\sim}{x}) - \lambda_k\|\underset{\sim}{h}\|F'(\underset{\sim}{x}))/\lambda_k^2\|\underset{\sim}{h}\|^2$$

$$= \frac{|F'(\underset{\sim}{x})|}{\lambda_k\|\underset{\sim}{h}\|}(1 - \psi(\underset{\sim}{x}, \underset{\sim}{h}, \lambda_k)) \quad . \tag{3.3}$$

λ_{k+1} is now found by minimizing $\phi_k(\lambda)$, and this gives

$$\lambda_{k+1} = |F'(\underset{\sim}{x})|/2C_k\|\underset{\sim}{h}\| \quad . \tag{3.4}$$

(ii) If λ_k fails (1.4) with $k > 0$ then λ_{k+1} is determined by applying a step of the secant algorithm to $\psi(\underset{\sim}{x}, \underset{\sim}{h}, \lambda) - 1/2$ using λ_k and the smallest value of λ which has previously failed (1.3).

To show that termination is guaranteed we note that in the second part of the method we are applying a standard root finding algorithm in a well behaved situation and with a tolerance of $1/2 - \sigma$ on the function value. Thus we concentrate on the first part and note that it is only necessary to show that the λ_k are decreasing fast enough for then (1.3) will be satisfied in a finite number of steps for each $\underset{\sim}{x}, \underset{\sim}{h}$. We have from (3.3) and (3.4) that

$$\lambda_{k+1} = \frac{\lambda_k}{2(1 - \psi(\underset{\sim}{x}, \underset{\sim}{h}, \lambda_k))}$$

$$< \frac{\lambda_k}{2(1 - \sigma)} \tag{3.5}$$

if the test (1.3) fails for $\lambda = \lambda_k$. Thus the worst possible situation is one in which the procedure finds a value of λ small enough to satisfy (1.3) by essentially repeated bisection. Note that by (3.3) and (3.4) C_k and λ_{k+1} are well determined quantities in this phase of the algorithm.

To show that the use of quadratic interpolation is efficient we write $\psi(\underset{\sim}{x}, \underset{\sim}{h}, \lambda_{k+1})$ in the form

$$\psi(\underset{\sim}{x}, \underset{\sim}{h}, \lambda_{k+1}) = -\frac{\lambda_{k+1}\|\underset{\sim}{h}\|F'(\underset{\sim}{x}) - \lambda_{k+1}^2\|\underset{\sim}{h}\|^2\int_0^1 (1-s)F''(\underset{\sim}{x} + (\lambda_{k+1}\underset{\sim}{h})s)\,ds}{-\lambda_{k+1}\|\underset{\sim}{h}\|F'(\underset{\sim}{x})}$$

$$= 1 - \frac{\lambda_{k+1}\|\underset{\sim}{h}\|}{|F'(\underset{\sim}{x})|}\int_0^1 (1-s)F''(\underset{\sim}{x} + (\lambda_{k+1}\underset{\sim}{h})s)\,ds$$

$$= 1 - \frac{1}{2C_k}\int_0^1 (1-s)F''(\underset{\sim}{x} + (\lambda_{k+1}\underset{\sim}{h})s)\,ds \tag{3.6}$$

$$= 1 - \frac{1}{2}\,\frac{\int_0^1 (1-s)F''(\underset{\sim}{x} + (\lambda_{k+1}\underset{\sim}{h})s)\,ds}{\int_0^1 (1-s)F''(\underset{\sim}{x} + (\lambda_k\underset{\sim}{h})s)\,ds}$$

or, introducting mean values $\underset{\sim}{\eta}_k$, $\underset{\sim}{\eta}_{k+1}$, as

$$\psi(\underset{\sim}{x}, \underset{\sim}{h}, \lambda_{k+1}) = 1 - \frac{1}{2}\,\frac{F''(\underset{\sim}{x} + \underset{\sim}{\eta}_{k+1})}{F''(\underset{\sim}{x} + \underset{\sim}{\eta}_k)} \quad . \tag{3.7}$$

This shows that if F is quadratic then $\psi(\underset{\sim}{x}, \underset{\sim}{h}, \lambda_1) = 1/2$ so that never more than one iteration is required in this case. The integral formula suggests that the local behaviour of F'' will have to be fairly extreme before (1.3) fails repeatedly. For, if the mean values can be estimated by the corresponding ordinates for the 1 point Gauss rule with $(1-s)$ as weight function then this gives $\underset{\sim}{\eta}_k = \frac{1}{3}\lambda_k\underset{\sim}{h}$. Thus each iteration significantly decreases the effective interval length and increases strongly the chance that the local approximating quadratic will be adequate.

4. An application to minimum norm problems.

Among generalizations of the Goldstein test one of the more interesting has been to minimum norm problems [5]. Let $\|\cdot\|$ denote a vector norm and set

$$F(\underset{\sim}{x}) = \|\underset{\sim}{f}(\underset{\sim}{x})\| \tag{4.1}$$

with $\dim \underset{\sim}{f} = n \geq p = \dim \underset{\sim}{x}$. The analogue of the Gauss-Newton algorithm generates a descent direction by solving the linear subproblem

$$\min_{\underset{\sim}{h}} \|\underset{\sim}{r}\|, \quad \underset{\sim}{r} = \nabla\underset{\sim}{f}(\underset{\sim}{x})\underset{\sim}{h} + \underset{\sim}{f}(\underset{\sim}{x}) \quad . \tag{4.2}$$

To generalize the Goldstein test we again compare the reduction in $F(\underset{\sim}{x})$ with the reduction achieved in the linear case, and this yields a procedure valid even if $\|\cdot\|$ is not continuously differentiable (the case of polyhedral norms for example). Thus we consider

$$\psi(\underset{\sim}{x}, \underset{\sim}{h}, \lambda) = \frac{\|\underset{\sim}{f}(\underset{\sim}{x})\| - \|\underset{\sim}{f}(\underset{\sim}{x} + \lambda\underset{\sim}{h})\|}{\lambda\{\|\underset{\sim}{f}(\underset{\sim}{x})\| - \min\limits_{\underset{\sim}{h}} \|\underset{\sim}{r}\|\}} \tag{4.3}$$

Provided $\|\underset{\sim}{h}\|$ is bounded (this is not guaranteed) then the Goldstein test forces convergence to a point at which

$$\|\underset{\sim}{f}(\underset{\sim}{x})\| = \min_{\underset{\sim}{h}} \|\underset{\sim}{r}\| \tag{4.4}$$

and such points are appropriately called stationary points [5].

Specializing the norm to the ℓ_2 norm it is convenient to take F as $\|\underset{\sim}{f}\|^2$ and to make the obvious changes to (4.3). In this case the result corresponds exactly to (1.2). We have

$$\nabla F(\underset{\sim}{x}) = 2\underset{\sim}{f}(\underset{\sim}{x})^T \nabla\underset{\sim}{f}(\underset{\sim}{x}) \tag{4.5}$$

and

$$\underset{\sim}{h} = -\nabla\underset{\sim}{f}(\underset{\sim}{x})^+ \underset{\sim}{f}(\underset{\sim}{x}) \tag{4.6}$$

so that a limit point $\underset{\sim}{x}^*$ of this variant of the Gauss-Newton algorithm is a point such that

$$0 = \lim_{i\to\infty} \nabla F(\underset{\sim}{x}_i)\underset{\sim}{h}_i = \lim_{i\to\infty} -2\underset{\sim}{f}(\underset{\sim}{x}_i)^T\nabla\underset{\sim}{f}(\underset{\sim}{x}_i)\nabla\underset{\sim}{f}(\underset{\sim}{x}_i)^+ \underset{\sim}{f}(\underset{\sim}{x}_i)$$

$$= \lim_{i\to\infty} -2\|P(\underset{\sim}{x}_i)\underset{\sim}{f}(\underset{\sim}{x}_i)\|^2$$

where $P(\underset{\sim}{x}_i)$ is the projector onto the range space of $\nabla\underset{\sim}{f}(\underset{\sim}{x}_i)$. Provided $\|\underset{\sim}{h}_i\|$ is bounded it follows that if $n = p$ and $\nabla\underset{\sim}{f}(\underset{\sim}{x}_i)$ has full rank for each i then $P(\underset{\sim}{x}_i) = I$ and $0 = \lim_{i\to\infty} \|\underset{\sim}{f}(\underset{\sim}{x}_i)\|$. Thus the Newton algorithm is convergent to a solution even if $\underset{\sim}{x}^*$ is an isolated singular point of $\nabla\underset{\sim}{f}(\underset{\sim}{x})$.

<u>Remark</u> (i). In this case the condition $\|\underset{\sim}{h}\|$ bounded is necessary. For consider $f = 1 + x^2$. We have $\nabla f = 2x$ and $h = -(1 + x^2)/2x$. Thus $\psi = 1 - \lambda\left(\frac{1+x^2}{4x^2}\right)$ and $x := x(1 - \frac{\gamma}{2})$ if $\lambda = \frac{\gamma x^2}{1+x^2}$. The Goldstein test is satisfied if $4(1-\sigma) \geq \gamma \geq 4\sigma$, and the resulting sequence of x iterates converges to zero which minimizes $\|1 + x^2\|$. This is a case in which $\{\lambda_i\} \to 0$ and the argument of section 2 shows that indeed $F' \to 0$ as $\lambda h = \frac{\gamma}{2} x \to 0$. However $\nabla Fh = -(1 + x^2) \not\to 0$. Note that $\min_{\underset{\sim}{h}} \|\underset{\sim}{r}\|$ is discontinuous at $x = 0$ so that $\|\underset{\sim}{f}\| = \min_{\underset{\sim}{h}} \|\underset{\sim}{r}\|$ is satisfied at the minimum although $\|\underset{\sim}{f}\| - \min_{\underset{\sim}{h}} \|\underset{\sim}{r}\| = \|\underset{\sim}{f}\| = 1 + x^2$ $\forall x \neq 0$.

(ii) It is readily verified that in the region of second order convergence the choice $\lambda_0 = 1$ will satisfy (1.3).

(iii) Note that (4.3) can be applied in cases in which derivatives are not available provided care is taken to ensure that $\underset{\sim}{h}$ is downhill. For example, if quasi Newton updates are used to estimate $\nabla\underset{\sim}{f}(\underset{\sim}{x})$ then we can show convergence to a stationary point $\underset{\sim}{x}^*$ of $F(\underset{\sim}{x})$ provided the appropriate Jacobian converges to $\nabla\underset{\sim}{f}(\underset{\sim}{x}^*)$. An algorithm of this kind has been realized by using a method of special iterations due to Powell [6] to force this convergence.

5. <u>Numerical experience.</u>

The procedure described here for satisfying the tests (1.3) and (1.4) has been coded in an implementation of Fletcher's 1970 algorithm for the minimization of an unconstrained function using conjugate direction methods [2] made by Michael Saunders and the author. This algorithm is described in [4]. It used product form updating of the Hessian estimate which was stored as the upper triangular factorization of its Choleski decomposition. The resulting algorithm has been in regular use as the main unconstrained optimization subroutine using derivative information in the subroutine library at the Australian National University for some six years. The line search has proved a very satisfactory part of the algorithm, and it seems

most unusual for more than one or two function evaluations to be made in this part of the calculation. It is unusual for the test (1.4) to fail once (1.3) has succeeded for the first time. However, it does happen occasionally but the strategy based on the secant algorithm handles this contingency very adequately. One of the considerations in writing the algorithm in the first place was that it be suitable for minimizing barrier and penalty objective functions, and, presumably, these have provided it with quite a severe test.

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